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SUBJECT: RESEARCH NOTES

IMPLEMENTING THE MONTE CARLO REDUCED SOURCE METHOD ON A SIMPLE 1-D PROBLEM

I. INTRODUCTION

The "reduced source" or "sequential Monte Carlo" iteration technique was first proposed by Halton[1,2] in 1962 for enhanced convergence of linear discrete systems. A single iteration of this approach was applied to continuous photon transport problems in 1974 by Fraley.[3] A decade later, Booth[4] outlined a few methods for implementing this iterative scheme to solve the continuous radiation transport equation. In this paper, we summarize the reduced source acceleration technique and apply it to a simple 1-D continuous transport problem.

The following is the time-independent neutron balance equation

$$\vec{\nu} \cdot \nabla N(\vec{r}, \vec{v}) + \Sigma_t(\vec{r}, \vec{v}) N(\vec{r}, \vec{v}) = \int \Sigma_s(\vec{r}, \vec{v'} \rightarrow \vec{v}) N(\vec{r}, \vec{v'}) d\vec{v'} + Q(\vec{r}, \vec{v}), \tag{1}$$

where

- $\vec{\nu}$—unit vector in the direction of the velocity;
- $\vec{v}$—velocity;
- N—transport flux;
- Q—source density;
- Σ_t—total cross section;
- Σ_s—scattering cross section.

Let

$$F(N) = \int \Sigma_s(\vec{r}, \vec{v'} \rightarrow \vec{v}) N(\vec{r}, \vec{v'}) d\vec{v'} - \vec{\nu} \cdot \nabla N(\vec{r}, \vec{v}) - \Sigma_t(\vec{r}, \vec{v}) N(\vec{r}, \vec{v}). \tag{2}$$

Equation (1.1) can be written as

$$F(N(\vec{r}, \vec{v})) + Q(\vec{r}, \vec{v}) = 0. \tag{3}$$

We are going to solve Eq. 3 (or Eq. 1) by the sequential Monte Carlo method. Pick an estimate of $N(\vec{r}, \vec{v})$, called $M(\vec{r}, \vec{v})$, such that

$$N(\vec{r}, \vec{v}) = M(\vec{r}, \vec{v}) + \phi(\vec{r}, \vec{v}),$$

where $\phi(\vec{r},\vec{v})$ is the difference in our estimate from the true solution. Putting this into Eq. 3 gives

$$F(\phi) + S(\vec{r},\vec{v}) = 0, \tag{4}$$

where

$$S(\vec{r},\vec{v}) = Q(\vec{r},\vec{v}) + F(M). \tag{5}$$

These equations can be solved in an iterative manner to obtain N. For the Hth iteration this gives

$$F(\phi^H) + S^H(\vec{r},\vec{v}) = 0, \tag{6}$$

where

$$S^H(\vec{r},\vec{v}) = Q(\vec{r},\vec{v}) + F(M^H) \tag{7}$$

and M is improved with each iteration according to

$$M^{H+1} = M^H + \phi^H.$$

Then, as $H \to \infty$, we should have

$$M^{H+1} \to N.$$

In the following sections, Eqs. 6 and 7 are applied to a one-dimensional problem, and convergence rates are reported for various discretization and flux expansion approaches.

II. A PROBLEM OF ONE DIMENSION WITHOUT SCATTERING

We consider here only the one-dimensional case in which there is no scattering and the source concentrates on x=0. Also, the energy is a constant and will be suppressed for simplicity.

In this simple case, M^H only depends on x and the functional $F(M^H)$ has the form

$$F(M^H) = -[\frac{d}{dx}M^H(x) + \Sigma_a M^H(x)]. \tag{8}$$

So, our problem can be formulated as

$$\begin{cases} \frac{dM^H}{dx} + \Sigma_a M^H = 0, & 0 < x \le T, \\ M^H(0) = Q_0, \end{cases} \tag{9}$$

where,Q_0 is the weight of the particle at $x = 0$. This very simple linear ODE Problem can be solved accurately. We are going to solve this problem by various techniques and compare the efficiency of all these techniques. As we will see, the crucial step is how to get an increment of the source from the previous stage because this will heavily influence the accuracy of the solution. Specifically, how do we evaluate $F(M^H)$ from Eq. 8?

We will test two ideas: one is discretizing the solution in the interval, the other is expanding the solution as a linear combination of the Legendre polynomials. We will see, by using the first idea, that we can only obtain the values of the solution at some discrete points of the interval; whereas by implementing the second idea, the solution can be expressed as a continuous function (actually, a polynomial).

III. DISCRETIZATION TECHNIQUES

In this section, we will test three different sampling methods to solve Eq. 9. All of these methods belong to the discretization category because they all need the solution to be discretized first. But the idea for solving the 0th stage is the same in all the three cases. We briefly describe it. The problem is

$$\begin{cases} \frac{d\phi^0}{dx} + \Sigma_a \phi^0 = 0, & 0 < x \leq T, \\ \phi^0(0) = Q_0, \end{cases} \tag{10}$$

First, discretize the interval $[0, T]$ (which can be considered as a line) into K_0 subintervals or zones and denote the nodes by $z_0, z_1, \ldots, z_{K_0}$ as in Fig. 1.

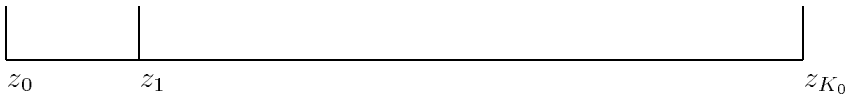

Figure 1: line

Now, we sample w particles with each having the weight Q_0. The initial points of the particles are all at z_0, and the length of track segments of the particles is decided by

$$l_n = -\log(\xi_n)/\Sigma_a$$

with $\xi_n \sim UNIF[0, 1]$, where $UNIF[0, 1]$ is the uniform distribution on $[0, 1]$. Then, the estimated value of the solution at z_k is

$$\phi^0(z_k) = Q_0 \frac{H(l_1 - z_k) + H(l_2 - z_k) + \cdots + H(l_w - z_k)}{w} \quad ,$$

where $H(x) = 1$ when $x \geq 0$ and 0 otherwise.

Now that we have the solution for the 0th stage, we will have the source for the first stage as we stated in the introduction. Let us formulate the problem for the first stage. With an initial guess $M^0(x) = 0$, then

$$M^1(x) = M^0(x) + \phi^0(x) = \phi^0(x)$$

and

$$M^2(x) = M^1(x) + \phi^1(x),$$

giving

$$\begin{aligned} \phi^1(0) &= M^2(0) - \phi^0(0) \\ &= Q_0 - Q_0 \\ &= 0. \end{aligned}$$

Thus, the problem for the first stage can be written as

$$\begin{cases} \frac{d\phi^1}{dx} + \Sigma_a \phi^1 = S^1(x), & 0 < x \leq T, \\ \phi^1(0) = 0. \end{cases} \tag{11}$$

The exact form of $S^1(x)$ will be described in the following three approaches.

A. *Approach 1.* Sampling the Position from the Source Function.

The best discretization results were obtained using this approach, as discussed in Section D.

First we divide $[0,T]$ into K subintervals (as shown in Fig. 1) with $z_k = x_k (k = 0, 1, \ldots, K)$ as the nodal points. The lengths of all the subintervals are equal to Δx.

Now, according to Eqs. 7 and 8, we get the source of the first stage by (note our initial guess $\mathrm{M}^0(x) = 0$, thus $\mathrm{M}^1(x) = \phi^0(x)$)

$$\begin{aligned} S^1(x) &= F(\phi^0) \\ &= -\{\frac{d\phi^0}{dx} + \Sigma_a \phi^0\}. \end{aligned}$$

Equation 11 gives a solution as follows

$$\begin{aligned} \phi^1(x) &= \int_0^x e^{-\Sigma_a(x-y)} S^1(y) dy \qquad (12) \\ &= \int_0^T |S^1(z)| dz \int_0^x e^{-\Sigma_a(x-y)} sign(S^1(y)) d(\frac{\int_0^y |S^1(z)| dz}{\int_0^T |S^1(z)| dz}) \\ &= \int_0^T |S^1(z)| dz \cdot \frac{1}{w} \sum_{n=1}^{w} e^{-\Sigma_a(x-t_n)} sign(S^1(t_n)), \end{aligned}$$

where

$$\xi_n \sim UNIF[0,1]$$

and t_n is defined by

$$\xi_n = \frac{\int_0^{t_n} |S^1(z)| dz}{\int_0^T |S^1(z)| dz}.$$

Now, just as we did for the 0th stage, by sampling the track segment we take away the exponential function. Let

$$\eta_m \sim UNIF[0,1],$$

and

$$r_{nm} = t_n - \ln(\eta_m)/\Sigma_a.$$

Thus, for any z_j, if we sample J times the track segments, we obtain the Monte Carlo approximation of the solution

$$\phi^1(z_j) = \frac{\int_0^T |S^1(z)| dz}{Jw} \sum_{n=1}^{w} \sum_{m=1}^{J} H(z_j - t_n) H(r_{nm} - z_j) sign(S^1(t_n)),$$

where $H(x) = 1$ for $x \geq 0$ and 0 otherwise. In our program, we chose J=1. From this expression, we can easily see that the computation of $\int_0^T |S^1(z)| dz$ would most probably influence the accuracy. So, we figured out the following way to evaluate this integral.

Recall that $S^1(x)$ is defined by

$$S^1(x) = -\{\frac{d\phi^0}{dx} + \Sigma_a \phi^0\}.$$

Then when K is sufficiently large, we will have

$$\begin{aligned}\int_0^T |S^1(z)|dz &\approx \sum_{k=1}^{K} |\int_{x_{k-1}}^{x_k} S^1(z)dz| \\ &= \sum_{k=1}^{K} |(\phi^0(x_k) - \phi^0(x_{k-1})) + \Sigma_a \int_{x_{k-1}}^{x_k} \phi^0(z)dz|.\end{aligned}$$

Thus, we can avoid evaluating the quotient of two infinitesimal quantities which leads to significant approximation. Furthermore, we reduce the error by using Simpson's rule to evaluate the integrals appearing in the sum.

We decide t_n in a similar way. Assume x_{k-1} and x_k are two neighboring points such that

$$\sum_{j=1}^{k-1} |\int_{x_{j-1}}^{x_j} S^1(z)dz| \le \xi_n \int_0^T |S^1(z)|dz < \sum_{j=1}^{k} |\int_{x_{j-1}}^{x_j} S^1(z)dz|.$$

Then, we chose $t_n = x_{k-1} + \zeta_n \Delta x$ with another $\zeta_n \sim UNIF[0,1]$.

Now, we have $\phi^1(x)$, so we can update the estimate $M^2 = M^1 + \phi^1$ and the source for the second stage becomes

$$S^2(x) = F(M^2),$$

where $F(M^2)$ can be treated in the same way as shown above for $F(M^1)$. Thus we can go to the second stage.

We can repeat this procedure as many times as we want and get the approximate solution of Eq. 9 by

$$N \approx M^{H+1} = \phi^0(x) + \phi^1(x) + \cdots + \phi^H(x).$$

To measure the accuracy and the convergence rate, we have to calculate some data beside the solution. We are mainly concerned with the estimated relative error, true relative error, and the variance. Take a point z_k(we took $z_k = T$). After Hth stages, the estimated and true relative error can be written as

$$EstErr(z_k) = \frac{\phi^H(z_k)}{N(z_k)}, \tag{13}$$

$$TrueErr(z_k) = \frac{N(z_k) - Sol(z_k)}{Sol(z_k)}, \tag{14}$$

where $Sol(z_k)$ is the value of the true solution at z_k.

For this approach, the variance of the estimation at x = T is

$$\begin{aligned}Var(\phi^H(T)) &= [\frac{1}{Jw} \sum_{n=1}^{w} \sum_{m=1}^{J} (H(T - t_n)H(r_{nm} - T)sign(S^H(t_n)) \int_0^T |S^H(z)|dz)^2 \\ &- (\phi^H(T))^2]/(Jw).\end{aligned}$$

B. *Approach 2.* Simple Difference.

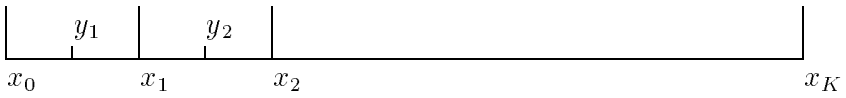

Figure 2: Slab

To get the source from the previous stage, we assume all the source in each subinterval concentrates on the middle point. So, $S^1(x)$ takes nontrivial values only at the points $y_k(k = 1, 2, \ldots, K)$. The values can be obtained by central difference, that is

$$S^1(y_k) = -\{\frac{\phi^0(x_k) - \phi^0(x_{k-1})}{x_k - x_{k-1}} + \Sigma_a \phi^0(y_k)\}. \tag{15}$$

Since we are only interested in the values of $\phi^1(x)$ at some discrete points $(x_0, x_1, \ldots, x_k)$, we have from Eq. 12

$$\begin{aligned}
\phi^1(x_k) &= e^{-\Sigma_a x_k} \int_0^{x_k} e^{\Sigma_a y} S^1(y) dy \\
&= e^{-\Sigma_a x_k} \sum_{j=1}^{k} \int_{x_{j-1}}^{x_j} e^{\Sigma_a y} S^1(y) dy \\
&\approx \sum_{j=1}^{k} \int_{x_{j-1}}^{x_j} e^{-\Sigma_a (x_k - y_j)} S^1(y_j) dy \\
&= \sum_{j=1}^{k} [S^1(y_j)\Delta x] e^{-\Sigma_a (x_k - y_j)} \\
&= \sum_{j=1}^{k} [S^1(y_j)\Delta x] e^{-\Sigma_a (k-j+0.5)\Delta x}.
\end{aligned}$$

Now, we construct k random variables $\xi_1, \xi_2, \ldots, \xi_k$, the probability distributions of which are as follows:

$$\begin{aligned}
\xi_1 : &\quad P(\xi_1 = S^1(y_1)\Delta x) = e^{-\Sigma_a (k-1+0.5)\Delta x}, \quad P(\xi_1 = 0) = 1 - e^{-\Sigma_a (k-1+0.5)\Delta x}; \\
\xi_2 : &\quad P(\xi_2 = S^1(y_2)\Delta x) = e^{-\Sigma_a (k-2+0.5)\Delta x}, \quad P(\xi_2 = 0) = 1 - e^{-\Sigma_a (k-2+0.5)\Delta x}; \\
&\quad \vdots \\
\xi_k : &\quad P(\xi_k = S^1(y_k)\Delta x) = e^{-\Sigma_a (k-k+0.5)\Delta x}, \quad P(\xi_k = 0) = 1 - e^{-\Sigma_a (k-k+0.5)\Delta x}.
\end{aligned}$$

Thus $\phi^1(x_k)$ can be expressed in a sum of the means of k independent random variables

$$\phi^1(x_k) = E[\xi_1] + E[\xi_2] + \cdots + E[\xi_k]. \tag{16}$$

It is somewhat different from $\phi^1(y_k)$ which can be written as

$$\begin{aligned}
\phi^1(y_k) &= e^{-\Sigma_a y_k}\int_0^{y_k} e^{\Sigma_a y}S^1(y)dy \\
&= e^{-\Sigma_a y_k}\sum_{j=1}^{k-1}\int_{x_{j-1}}^{x_j} e^{\Sigma_a y}S^1(y)dy + e^{-\Sigma_a y_k}\int_{x_{k-1}}^{y_k} e^{\Sigma_a y}S^1(y)dy \\
&\approx \sum_{j=1}^{k-1}\int_{x_{j-1}}^{x_j} e^{-\Sigma_a(y_k-y_j)}S^1(y_j)dy + e^{-\Sigma_a y_k+\Sigma_a\frac{y_k+x_{k-1}}{2}}S^1(y_k)\frac{\Delta x}{2} \\
&= \sum_{j=1}^{k-1}[S^1(y_j)\Delta x]e^{-\Sigma_a(k-j)\Delta x} + e^{-\Sigma_a\frac{\Delta x}{4}}\cdot[S^1(y_k)\cdot\frac{\Delta x}{2}].
\end{aligned}$$

We now construct our probabilistic model as follows. As for $\phi^1(x_k)$, we first write down the probability distributions:

$$\begin{array}{lll}
\xi_1: & P(\xi_1 = S^1(y_1)\Delta x) = e^{-\Sigma_a(k-1)\Delta x}, & P(\xi_1 = 0) = 1 - e^{-\Sigma_a(k-1)\Delta x}; \\
& \vdots & \\
\xi_{k-1}: & P(\xi_{k-1} = S^1(y_{k-1})\Delta x) = e^{-\Sigma_a(k-(k-1))\Delta x}, & P(\xi_{k-1} = 0) = 1 - e^{-\Sigma_a(k-(k-1))\Delta x}; \\
\xi_k: & P(\xi_k = e^{-\Sigma_a\frac{\Delta x}{4}}S^1(y_k)\frac{\Delta x}{2}) = 1, & P(\xi_k = 0) = 0.
\end{array}$$

Thus, we can still get a probabilistic model for $\phi^1(y_k)$

$$\phi^1(y_k) = E[\xi_1] + E[\xi_2] + \cdots + E[\xi_k]. \tag{17}$$

For the first stage, it seems much more difficult than for the 0th stage, but it can be solved in almost the same way. Now, we must keep in mind that we have K particles which concentrate on different positions, $S^1(y_1)\Delta x$ at y_1, $S^1(y_2)\Delta x$ at y_2, $\cdots$, $S^1(y_K)\Delta x$ at y_K. For each particle, track w (can be chosen arbitrarily, differently for different particles) times, then add the total for each point, and we are done with the first stage.

We can use Eqs. 13 and 14 (for H=1) to obtain the estimated and true relative errors. The variance is as follows.

For simplicity of the notations, we only write down the variance of each stage at the final point $x_K = T$. It is

$$Var(\phi^m(T)) = \sum_{k=1}^{K}\frac{\sigma_k^2}{n_k}, \tag{18}$$

where

$$\sigma_k^2 = [S^m(y_k)\Delta x]^2 e^{-\Sigma_a(K-k+0.5)\Delta x}(1 - e^{-\Sigma_a(K-k+0.5)\Delta x})$$

is the variance of sample of ξ_k, and n_k is the number of samples of ξ_k.

In the above, we intentionally wrote n_k to imply that we can choose a different number of samples for each particle. Actually, if we keep the number of samples for each stage fixed but carefully

choose n_k for each subinterval, then we can reduce the variance significantly, especially for a big K. We write down the result in the following but do not elaborate on it. Let

$$n = n_1 + n_2 + \cdots + n_K,$$

and

$$\alpha = \frac{1}{n}[\sum_{k=1}^{K} |S^m(y_k)\Delta x| e^{-\frac{\Sigma_a}{2}(K-k+0.5)\Delta x}(1 - e^{-\Sigma_a(K-k+0.5)\Delta x})^{\frac{1}{2}}].$$

If we take

$$n_k = \frac{|S^m(y_k)\Delta x|}{\alpha} e^{-\frac{\Sigma_a}{2}(K-k+0.5)\Delta x}(1 - e^{-\Sigma_a(K-k+0.5)\Delta x})^{\frac{1}{2}},$$

the variance of Eq. 18 will attain its minimum

$$Var_{min} = \frac{1}{n}(\sum_{k=1}^{K} \sigma_k)^2.$$

C. *Approach* 3. Sample Another Function.

Begin from Eq. 12 and use Fig. 1. We write down Eq. 12 in a different form

$$\phi^1(x) = f(x) \int_0^x S^1(y) g(y) dy,$$

where

$$f(x) = \int_0^x e^{-\Sigma_a(x-z)} dz = \frac{1}{\Sigma_a}(1 - e^{-\Sigma_a x}),$$

$$g(y) = \frac{\Sigma_a e^{-\Sigma_a(x-y)}}{1 - e^{-\Sigma_a x}}.$$

To estimate $\phi^1(x)$ by the Monte Carlo method, we sample

$$\xi_n \sim UNIF[0,1]$$

and solve

$$\xi_n = \int_0^{y_n} g(z) dz$$

for y_n,

$$y_n = \log(1 + \xi_n(e^{\Sigma_a x} - 1))/\Sigma_a.$$

Thus, if we sample w times, we get the estimation of $\phi^1(z_k)$ by

$$\begin{aligned} \phi^1(z_k) &= \frac{f(z_k)}{w} \sum_{n=1}^{w} S^1(y_n) \\ &= \frac{1}{w\Sigma_a}(1 - e^{-\Sigma_a z_k}) \cdot \sum_{n=1}^{w} S^1(y_n). \end{aligned}$$

Recall that $S^1(x)$ is a discrete function. We do not have the value $S^1(y_n)$ if y_n is not equal to any z_k. To overcome this difficulty, we use linear interpolation. If $z_{j-1} < y_n \leq z_j$, we use the approximation

$$S^1(y_n) \approx \frac{S^1(z_j)(y_n - z_{j-1}) + S^1(z_{j-1})(z_j - y_n)}{z_j - z_{j-1}}.$$

Thus, we estimate $\phi^1(z_k)$ by

$$\phi^1(z_k) = \frac{1}{w\Sigma_a}(1 - e^{-\Sigma_a z_k}) \cdot \sum_{n=1}^{w} \frac{S^1(z_j)(y_n - z_{j-1}) + S^1(z_{j-1})(z_j - y_n)}{z_j - z_{j-1}},$$

where $z_{j-1} < y_n \leq z_j$. We still use Eqs. 13 and 14 to estimate both the estimated and the true relative errors for each point z_k. But the formula for the variance is different. The variance for the estimation at $x = T$ is

$$\begin{aligned} Var(\phi^1(T)) &= [\frac{1}{w}\sum_{n=1}^{w}(\frac{1}{\Sigma_a}(1 - e^{-\Sigma_a T})\frac{S^1(z_j)(y_n - z_{j-1}) + S^1(z_{j-1})(z_j - y_n)}{z_j - z_{j-1}})^2 \\ &- (\phi^1(T))^2]/w. \end{aligned}$$

D. Comparison of Convergence Rates.

Finally, let us compare the results obtained by these three different approaches. We only compare the two important measures (estimated and true relative errors, see Eqs. 13 and 14) at the final point $x = T$. We chose $T = 5cm, Q_0 = 1, \Sigma_a = 1/cm$. In Table 1, the number of subintervals (K) is 100, and the number of particles per iteration or stage is 10,000. Data presented in the following tables is included only to the point where the estimated error exceeds the true error. While exponential convergence continues beyond this point, convergence is to the incorrect solution due to various approximations discussed in each approach.

Table 1.

Stages	Approach 1		Approach 2		Approach 3	
	Est. Error	True Error	Est. Error	True Error	Est. Error	True Error
0	1.0e+00	-5.6e-03	1.0e+00	-2.2e-01	1.0e+00	-2.2e-01
1	4.9e-02	4.5e-02	-2.0e-01	-1.8e-02	-2.2e-01	6.2e-03
2	-4.4e-02	1.0e-03	-1.6e-02	-1.5e-03	6.2e-03	-4.5e-05
3	-1.0e-03	-2.2e-05				
4	3.6e-05	1.3e-05				
5	-3.5e-05	-2.2e-05				

In Table 2, the number of subintervals is increased to 500, and the number of particles per iteration is still 10,000.

$Table\ 2.$

Stages	Approach 1		Approach 2		Approach 3	
	Est. Error	True Error	Est. Error	True Error	Est. Error	True Error
0	1.0e+00	-5.6e-03	1.0e+00	-2.2e-01	1.0e+00	-2.2e-01
1	1.0e-01	1.1e-01	-9.6e-02	-1.1e-01	-2.4e-01	2.2e-02
2	-1.2e-01	-7.0e-03	-8.0e-02	-2.8e-02	4.3e-02	-2.1e-02
3	1.9e-02	1.2e-02	-2.5e-02	-3.0e-03	-2.5e-02	4.0e-03
4	-1.2e-02	-1.2e-05	-3.4e-03	4.5e-04	1.5e-02	-1.1e-02
5	1.1e-04	9.6e-05			-1.7e-02	6.2e-03
6	7.4e-05	1.7e-04				
7	-1.7e-04	-2.2e-06				
8	2.9e-06	6.9e-07				
9	-1.7e-06	-9.6e-07				
10	7.3e-07	-2.3e-07				

From Table 1, we see that carefully handling the source from the previous stages will make a big difference for the final results. Besides, we can also get better results by increasing the number of the subintervals.

IV. FLUX EXPANSION TECHNIQUES

As the title implies, we will expand the flux according to some set of functions $E = \{e_0(x), e_1(x), e_2(x), \ldots\}$. The only requirement on E is that it must be complete, roughly speaking. In other words, we should have the equality

$$\phi(x) = \sum_{j=0}^{\infty} a_j e_j(x)$$

if $\phi(x)$ is continuous and differentiable. Here we chose $E = \{Legendre\ polynomials\}$. We will give three different sampling methods, but they are same for the 0th stage as in the case of the discretization technique.

Suppose

$$\phi^0(x) = \sum_{j=0}^{\infty} a_j P_j(f), \tag{19}$$

where, as in Ref. 4, $P_j(f)(j = 0, 1, 2, \ldots)$ are Legendre polynomials and $f = \frac{2x}{T} - 1$ (a variable transform) to ensure that when $x \in [0, T], f \in [-1, 1]$. Then

$$\begin{aligned} a_j &= \frac{2j+1}{2} \int_{-1}^{1} \phi^0(x) P_j(f) df \\ &= \frac{2j+1}{T} \int_0^T \phi^0(x) P_j(\frac{2x}{T} - 1) dx, j = 0, 1, 2, \cdots. \end{aligned} \tag{20}$$

Now, we use the Monte Carlo method to estimate a_j. From Eq. 10 which $\phi^0(x)$ satisfies, we know that the source particles appear only at $x = 0$, and along each track segment of the particle, $\phi^0(x) \equiv Q_0$. Now, let us first write down the length of each track segment that is sampled by the following method. Suppose

$$\xi_n \sim UNIF[0,1], \tag{21}$$

and let

$$X_n = -\log(\xi_n)/\Sigma_a, \tag{22}$$
$$Y_n = \min\{T, X_n\},$$

where $n = 1, 2, \ldots, w$. Then we have the estimated value of a_j

$$a_j = \frac{2j+1}{T} Q_0 \frac{1}{w} \sum_{n=1}^{w} \int_0^{Y_n} P_j(\frac{2x}{T} - 1)dx. \tag{23}$$

Now, we list some useful formulae about Legendre polynomials without proof. Please refer to Ref 5.

$$P_j(f) = \frac{1}{2j+1}(P'_{j+1}(f) - P'_{j-1}(f)),$$
$$P'_j(f) = (2j-1)P_{j-1}(f) + (2j-5)P_{j-3}(f) + (2j-9)P_{j-5}(f) + \ldots,$$
$$P_j(1) = 1, \qquad P_j(-1) = (-1)^j,$$
$$\int_{-1}^{1} P_j(f)P_k(f)df = \begin{cases} 0, & j \neq k, \\ \frac{2}{2j+1}, & j = k. \end{cases}$$

where, $j, k = 0, 1, 2, \ldots, and \;\; P_{-1}(f) \equiv 0$. These formulae will be used to evaluate Eq. 23 and some later integrals.

Before we switch to the first stage, we write down the source $S^1(x)$. According to Eq. 8,

$$F(\phi^0) = -\{\frac{d\phi^0}{dx} + \Sigma_a \phi^0\},$$

and

$$S^1(x) = F(\phi^0).$$

Since ϕ^0 is continuously defined, therefore $F(\phi^0)$ can be obtained in an accurate way. We must note that, when we use Eq. 19 to express $\phi^0(x)$, we can only use a finite sum. Thus, $\phi^0(x)$ is actually a polynomial. Now the problem for the first stage can be formulated as

$$\begin{cases} \frac{d\phi^1}{dx} + \Sigma_a \phi^1 = S^1(x), & 0 < x \leq T, \\ \phi^1(0) = Q_0 - \phi^0(0). \end{cases} \tag{24}$$

Note, $\phi^1(0) \neq 0$ in general. To solve this problem, we split it into two problems first:

$$\begin{cases} \frac{d\phi_1^1}{dx} + \Sigma_a \phi_1^1 = 0, & 0 < x \leq T, \\ \phi_1^1(0) = Q_0 - \phi^0(0). \end{cases}$$

and second:

$$\begin{cases} \frac{d\phi_2^1}{dx} + \Sigma_a \phi_2^1 = S^1(x), \quad 0 < x \leq T, \\ \phi_2^1(0) = 0. \end{cases} \tag{25}$$

The first problem can be solved for $\phi_1^1(x)$ in the same way as for the 0th stage. If we can solve Eq. 25 for $\phi_2^1(x)$, then $\phi^1(x) = \phi_1^1(x) + \phi_2^1(x)$ is the solution of Eq. 24 by the principle of superposition. To solve Eq. 25, we consider the following problem

$$\begin{cases} \frac{d\psi}{dx} + \Sigma_a \psi = 0, \qquad 0 < y < x \leq T, \\ \psi(x,y)|_{x=y} = S^1(y), \end{cases} \tag{26}$$

where y is considered as a parameter. The following lemma constructs a relation between the solution of Eq. 25 and that of Eq. 26.

$Lemma.$ If $\psi = \psi(x,y)$ is the solution of Eq. 26, then

$$\phi_2^1(x) = \int_0^x \psi(x,y)dy$$

is the solution of Eq. 25.

Now, we expand $\phi_2^1(x)$ in terms of $P_j(f)$'s.

$$\phi_2^1 = \sum_{j=0}^{\infty} a_j P_j(f).$$

Then

$$\begin{aligned} a_j &= \frac{2j+1}{T} \int_0^T \phi_2^1(x) P_j(\frac{2x}{T} - 1)dx \\ &= \frac{2j+1}{T} \int_0^T [\int_0^x \psi(x,y)dy] P_j(\frac{2x}{T} - 1)dx \\ &= \frac{2j+1}{T} \int_0^T [\int_y^T \psi(x,y) P_j(\frac{2x}{T} - 1)dx]dy. \end{aligned}$$

Therefore, we can consider $\psi(x,y)$ as the flux with the source particles $S^1(y)$ only at $x = y$, and along each track segment starting from y, $\psi(x,y) \equiv S^1(y)$. Thus, if we assume ξ_n and X_n are defined by Eq. 21 and Eq. 22, and

$$Y_n = \min\{T, X_n + y\}, \tag{27}$$

then we have the estimations of a_j's as follows

$$\begin{aligned} a_j &= \frac{1}{w} \sum_{n=1}^{w} [\frac{2j+1}{T} \int_0^T S^1(y)dy \int_y^{Y_n} P_j(\frac{2x}{T} - 1)dx]. \\ &= \frac{1}{w} \sum_{n=1}^{w} I_{jn}, \end{aligned} \tag{28}$$

where

$$I_{jn} = \frac{2j+1}{T} \int_0^T S^1(y)dy \int_y^{Y_n} P_j(\frac{2x}{T} - 1)dx. \tag{29}$$

Now, we have three different approaches to evaluate Eq. 29. We will describe them one by one.

A. *Approach 1.* Discretizing the Integral about y.

Divide [0,T] into K subintervals

$$[x_0, x_1],\ [x_1, x_2],\ \ldots, [x_{K-1}, x_K].$$

Then we use the following formulae to estimate a_j:

$$a_j = \frac{2j+1}{T} \sum_{k=1}^{K} \int_{x_{k-1}}^{x_k} S^1(y)dy \cdot \frac{1}{w} \sum_{n=1}^{w} [\int_{y_k}^{Y_n} P_m(\frac{2x}{T} - 1)dx], \tag{30}$$

where

$$y_k = \frac{x_{k-1} + x_k}{2}.$$

Equation 30 is straightforward; nothing needs to be explained. We use the following formulae to calculate the estimated and true relative errors.

$$EstErr(x) = \frac{\phi^1(x)}{N(x)}, \tag{31}$$

$$TruErr(x) = \frac{N(x) - Sol(x)}{Sol(x)}, \tag{32}$$

where $Sol(x)$ is the value of the true solution at x. The variances for estimating a coefficient a_j can be evaluated by

$$Var(a_j) = [\frac{1}{w} \sum_{n=1}^{w} (\frac{2j+1}{T} \sum_{k=1}^{K} \int_{x_{k-1}}^{x_k} S^1(y)dy \int_{y_k}^{Y_n} P_m(\frac{2x}{T} - 1)dx)^2 - (a_j)^2]/w.$$

Thus, the variance of estimating the value of the solution at T is

$$Var(\phi^1(T)) = \sum_{j=0}^{n_0-1} Var(a_j) + Var(\phi_1^1(T)). \tag{33}$$

B. *Approach 2.* Sample the Initial Position from $S^1(y)$.

First, we write down a_j in a convenient form

$$\begin{aligned} a_j &= \frac{1}{w} \sum_{n=1}^{w} \frac{2j+1}{T} \int_0^T S^1(y)dy \int_y^{Y_n} P_j(\frac{2x}{T} - 1)dx \\ &= \frac{1}{w} \sum_{n=1}^{w} \int_0^T S^1(y) Q_j(y)dy, \end{aligned}$$

where

$$Q_j(y) = \frac{2j+1}{T} \int_y^{Y_n} P_j(\frac{2x}{T} - 1)dx.$$

Now, we describe how to estimate

$$I_j = \int_0^T S^1(y) Q_j(y)dy.$$

Assume $S^1(y) \neq 0$. Then

$$I_j = (\int_0^T |S^1(z)|dz)[\int_0^T Q_j(y) sign(S^1(y)) d(\frac{\int_0^y |S^1(z)|dz}{\int_0^T |S^1(z)|dz})].$$

Construct a density function as follows

$$g(y) = \begin{cases} 0, & y < 0, \\ \frac{|S^1(y)|}{\int_0^T |S^1(z)|dz}, & 0 \leq y \leq T, \\ 0, & y > T. \end{cases}$$

Assume

$$\xi_m \sim UNIF[0,1].$$

Then for each ξ_m, there exists a unique y_m, such that

$$\xi_m = \int_0^{y_m} g(y)dy.$$

If we choose J samples, we can estimate I_j by

$$I_j = \frac{\int_0^T |S^1(z)|dz}{J} \sum_{m=1}^{J} Q_j(y_m) sign(S^1(y_m)).$$

In our program, we chose $J = 1$. The coefficient a_j is estimated by

$$a_j = \frac{\int_0^T |S^1(z)|dz}{wJ} \sum_{m=1}^{J} \sum_{n=1}^{w} \frac{2j+1}{T} sign(S^1(y_m)) \int_{y_m}^{Y_n} P_j(\frac{2x}{T} - 1)dx.$$

Equations 31 and 32 are still applicable here. The variances for a_j are

$$\begin{aligned} Var(a_j) &= (\int_0^T |S^1(z)|dz)^2 \cdot [\frac{1}{wJ} \sum_{m=1}^{J} \sum_{n=1}^{w} (\frac{2j+1}{T} sign(S^1(y_m)) \\ &\cdot \int_{y_m}^{Y_n} P_j(\frac{2x}{T} - 1)dx)^2 - (\frac{1}{wJ} \sum_{m=1}^{J} \sum_{n=1}^{w} \frac{2j+1}{T} sign(S^1(y_m)) \\ &\cdot \int_{y_m}^{Y_n} P_j(\frac{2x}{T} - 1)dx)^2]/(Jw). \end{aligned}$$

The variance for the solution at T is

$$Var(\phi^1(T)) = \sum_{j=0}^{n_0-1} Var(a_j) + Var(\phi_1^1(T)).$$

C. *Approach* 3. Evaluate Eq. 29 Accurately.

This can be done by using those formulae listed after Eq. 23. However, this may not be a good idea because we have to do many integrations by parts, especially when many polynomials are

involved. To make it easy to implement by the programming code, we do some calculations on Eq. 29. Remember $f = \frac{2x}{T} - 1$. We have

$$\begin{aligned} I_{jn} &= \frac{2j+1}{2}\int_0^T S^1(y)dy \int_{\frac{2y}{T}-1}^{\frac{2Y_n}{T}-1} P_j(f)df \\ &= \frac{1}{2}\int_0^T S^1(y)dy \int_{\frac{2y}{T}-1}^{\frac{2Y_n}{T}-1} (P'_{j+1}(f) - P'_{j-1}(f))df \\ &= \frac{1}{2}\int_0^T S^1(y)(P_{j+1}(\frac{2Y_n}{T}-1) - P_{j-1}(\frac{2Y_n}{T}-1))dy \\ &- \frac{1}{2}\int_0^T S^1(y)(P_{j+1}(\frac{2y}{T}-1) - P_{j-1}(\frac{2y}{T}-1))dy \\ &\equiv I^1 - I^2. \end{aligned}$$

I^2 can be evaluated easily. To evaluate I^1, we need to consider two cases:

(a) $X_n \geq T$. Then $Y_n = T$. So,

$$I_1 = \frac{1}{2}\int_0^T S^1(y)(P_{j+1}(1) - P_{j-1}(1))dy;$$

(b) $X_n < T$. We have

$$\begin{aligned} I^1 &= \frac{1}{2}\int_0^{T-X_n} S^1(y)(P_{j+1}(\frac{2(X_n+y)}{T}-1) - P_{j-1}(\frac{2(X_n+y)}{T}-1))dy \\ &+ \frac{1}{2}(P_{j+1}(1) - P_{j-1}(1))\int_{T-X_n}^T S^1(y)dy. \end{aligned}$$

The second integral is easily calculated, but the first will cost many hours of computer time.

The formulae in Eq. 31 and Eq. 32 can still be used to evaluate the estimated and the true relative errors. But the variances for calculating the coefficient a_j can be evaluated by

$$Var(a_j) = [\frac{1}{w}\sum_{n=1}^{w}(\frac{2j+1}{T}\int_0^T S^1(y)dy \int_y^{Y_n} P_j(\frac{2x}{T}-1)dx)^2 - (a_j)^2]/w.$$

Thus, the variance for estimating the solution at T can be written as follows

$$Var(\phi^1(T)) = \sum_{j=0}^{n_0-1} Var(a_j) + Var(\phi_1^1).$$

D. Comparison of Cnvergence Rates.

Finally, let us compare the numerical results obtained by these different sampling methods. It is clear that the number of polynomials we use will be a crucial part of the final results. As in the discrete case, we chose $T = 5cm$, $\Sigma_a = 1/cm$, and $Q_0 = 1$. Also, we chose the number of the particles per iteration to be 10,000. Table 3 lists the results using the first ten Legendre polynomials.

Table 3.

Stages	Approach 1		Approach 2		Approach 3	
	Est. Error	True Error	Est. Error	True Error	Est. Error	True Error
0	1.0e+00	-1.7e-01	1.0e+00	-1.7e-01	1.0e+00	-1.7e-01
1	-1.6e-01	-5.0e-03	-1.8e-01	9.0e-03	-1.7e-01	-3.5e-04
2	-1.8e-04	-4.8e-03	8.7e-03	3.2e-04	-5.1e-04	1.6e-04
3	-4.1e-03	-6.7e-04	1.5e-04	1.6e-04		
4	-1.5e-03	8.6e-04				
5	7.6e-04	1.0e-04				

In Table 4, the number of Legendre coefficients is increased to 20. This table lists results only for Approaches 1 and 2, since Approach 3 required too much CPU time for 10,000 particles per iteration.

Table 4.

Stages	Approach 1		Approach 2	
	Est. Error	True Error	Est. Error	True Error
0	1.00e+00	-2.37e-01	1.00e+00	-2.37e-01
1	-2.72e-01	2.77e-02	-2.28e-01	-6.99e-03
2	3.03e-02	-2.66e-03	-5.91e-03	-1.07e-03
3	-1.17e-03	-1.50e-03	-1.30e-03	2.24e-04
4	-1.98e-03	4.80e-04	2.32e-04	-8.32e-06
5	5.41e-04	-6.13e-05	-8.67e-06	3.50e-07
6	-4.99e-05	-1.14e-05	4.41e-07	-9.10e-08
7	-1.02e-05	-1.22e-06	-9.54e-08	4.42e-09
8	-1.15e-06	-7.18e-08	4.87e-09	-4.47e-10
9	-6.72e-08	-4.61e-09	-4.74e-10	2.68e-11
10	-5.59e-09	9.80e-10	2.93e-11	-2.58e-12
11	1.52e-09	-5.39e-10	-2.81e-12	2.29e-13
12	-4.43e-10	-9.66e-11	2.33e-13	-3.86e-15
13	-9.28e-11	-3.86e-12	-9.35e-15	5.54e-15
14	-3.70e-12	-1.62e-13		
15	1.49e-13	-3.11e-13		
16	-2.93e-13	-1.79e-14		
17	-2.46e-14	6.69e-15		

From these two cases, it is easily seen that we can improve the results dramatically by increasing the number of the Legendre polynomials used for expanding the flux. From the following simple example, we know that the results are not very sensitive to the number of the particles.

The following table lists an example for Approach 3 with 16 Legendre polynomials and only 100 particles per iteration. The other parameters are the same as discussed above.

Table 5.

Stages	Approach 3	
	Est. Error	True Error
0	1.00e+00	1.48e+00
1	1.32e+00	-4.87e-01
2	-4.86e-01	-4.66e-04
3	-1.54e-03	1.07e-03
4	1.15e-03	-8.08e-05
5	-1.18e-04	3.77e-05
6	3.75e-05	1.51e-07
7	4.57e-08	1.06e-07
8	1.07e-07	-9.72e-10
9	-1.55e-09	5.76e-10
10	4.69e-10	1.07e-10

V. SUMMARY AND FUTURE WORK

In this report, we have discussed two main techniques to address the one-dimensional transport problem without scattering. We used some different sampling methods to construct some mathematical models and related computer programs.

First for the discretization methods, we know it is crucial to get the source from the previous stages. So, any effort to reduce the source error will definitely make sense for solving the problem more accurately. Besides, sampling different distribution functions, or generally, using importance sampling in our problem probably will improve the results very much.

Compared to the discretization methods, the flux expansion techniques look much more encouraging. It improves the results significantly, and besides, it gives us a continuously defined function which would provide more knowledge than the discretization methods do.

Our future work is to apply those methods, both discretization and flux expansion techniques, to multidirectional-scattering and multidimensional problems. We are also interested in developing some new methods in solving these problems.

REFERENCES

[1] J. H. Halton, “Sequential Monte Carlo,” Proc.Camb. Phil. Soc., Vol. 58, pp. 57-78 (1962).

[2] J. H. Halton, “Sequential Monte Carlo Techniques for the Solution of Linear Systems,” Jour. Sci. Comp., Vol. 9, No. 2, pp. 213-257 (1994).

[3] G. S. Fraley et al., “Thermonuclear Burn Characteristics of Compressed Deuterium-Tritium Microspheres,” Phys. Fluids, Vol. 17, No. 2, pp. 474-489, App. B (1974).

[4] R. A. Forster et al., “Radiation Transport,” LA–110465–PR, Los Alamos National Laboratory progress report (1984).

[5] T. M. Macrobert, “Spherical Harmonics,” Pergamon Press (1967).

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